

chain nodes :

11 12 15 19 20 21 22 24 25 26 27

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

10-11 11-12 12-15 19-25 20-22 20-21 20-26 21-24 25-26 25-27

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 8-9 9-10

exact/norm bonds :

2-7 3-10 7-8 8-9 9-10 12-15 19-25 20-22 20-21 21-24 25-27

exact bonds :

10-11 11-12 20-26 25-26

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:N,NH,Hy

G2:CH2,NH,O,SO2,S

G3:H,Ak,Cb

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:CLASS 12:CLASS 15:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 24:CLASS

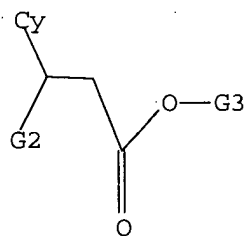
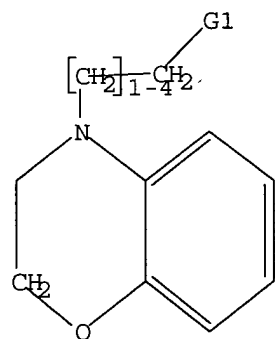
25:CLASS 26:CLASS 27:Atom

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 N,NH,Hy

G2 CH2,NH,O,SO2,S

G3 H,Ak,Cb

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 16:31:59 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 205 TO ITERATE

100.0% PROCESSED 205 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 3241 TO 4959  
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 16:32:07 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 4376 TO ITERATE

100.0% PROCESSED 4376 ITERATIONS 48 ANSWERS  
SEARCH TIME: 00.00.01

L3 48 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	161.54

FILE 'CAPLUS' ENTERED AT 16:32:12 ON 18 NOV 2005  
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FILE COVERS 1907 - 18 Nov 2005 VOL 143 ISS 22  
FILE LAST UPDATED: 17 Nov 2005 (20051117/ED)

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=> s l3

L4 1 L3

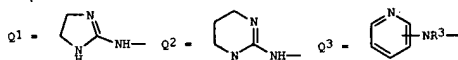
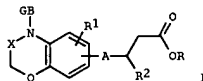
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own work

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2003:300614 CAPLUS  
 DOCUMENT NUMBER: 138:321293  
 TITLE: Preparation of benzoxazines as integrin antagonists  
 INVENTOR(S): Vianello, Paola; Bandiera, Tiziano  
 PATENT ASSIGNEE(S): Pharmacia & Upjohn, S.P.A., Italy  
 SOURCE: U.S. Pat. Appl. Publ., 31 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003073688	A1	20030417	US 2001-924709	20010808
US 6750215	B2	20040615		
US 2004224948	A1	20041111	US 2004-821104	20040408
			US 2001-924709	A1 20010808

PRIORITY APPL. INFO.: MARPAT 138:321293  
 OTHER SOURCE(S): GI



AB Title compds. [I; g = Q'NHC(Q)NH, Q1, Q2, Q3, etc.; Q = NH, O; Q' = H alkyl, Ph, phenylalkyl; R3 = H, alkyl; B = (CH2)m(CH:CH)pY; m = 1-3; p = 0, 1; Y = CH2, CO; R = H, alkyl, alkenyl, alkynyl, aryl, aralkyl; R1 = H, alkyl, alkoxy, OH, halo, CF3; R2 = alkyl, alkenyl, alkynyl, aryl, (substituted) heteroaryl; A = CH2, NH, O, S, SO, SO2], were prepared Thus, 7-nitro-3-oxo-3,4-dihydro-2H-1,4-benzoxazine (preparation given) in THF/DMF

at 0° was treated with potassium hexamethyldisilazide and then with 3-[N-benzoyloxycarbonyl-N-(1-oxido-2-pyridinyl)amino]propyl methanesulfonate in THF followed by heating at 80° for 3 h to give 34% 7-nitro-4-[3-(N-benzoyloxycarbonyl-N-(1-oxido-2-pyridinyl)amino)propyl]-3-oxo-3,4-dihydro-2H-1,4-benzoxazine. This was stirred with TiCl4 and SnCl2 in THF/EtOH for 6 h at 40° to give 70% 7-amino-4-[3-(N-benzoyloxycarbonyl-N-(2-pyridinyl)amino)propyl]-3-oxo-3,4-dihydro-2H-1,4-benzoxazine. The latter was converted in several steps to title compound N-[3-oxo-4-[3-(2-pyridinylamino)propyl]-3,4-dihydro-2H-1,4-benzoxazin-7-yl]-3-phenyl-L-alanine (II). II bound to  $\alpha v \beta 3$  vitronectin receptors with IC50 = 0.011  $\mu$ M. A II capsule formulation is given.

IT 511544-45-9P 511544-47-1P 511544-50-6P

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

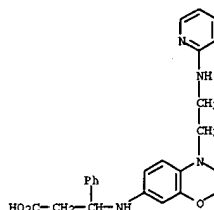
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 511545-37-2P 511545-39-4P 511545-40-7P  
 511545-42-9P 511545-44-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

RN (prepn. of benzoxazines as integrin antagonists)

RN 511544-45-9 CAPLUS

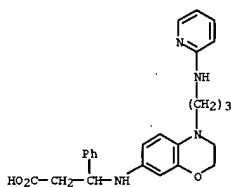
CN Benzenepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[2-(2-pyridinylamino)ethyl]-2H-1,4-benzoxazin-7-yl]amino]- (9CI) (CA INDEX NAME)



RN 511544-47-1 CAPLUS

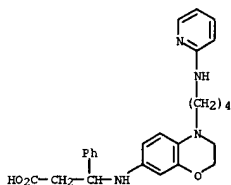
CN Benzenepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[3-(2-pyridinylamino)propyl]-2H-1,4-benzoxazin-7-yl]amino]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



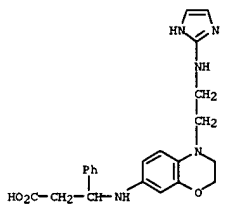
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CN Benzenepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[4-(2-pyridinylamino)butyl]-2H-1,4-benzoxazin-7-yl]amino]- (9CI) (CA INDEX NAME)



RN 511544-52-8 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[2-(1H-imidazol-2-ylamino)ethyl]-2H-1,4-benzoxazin-7-yl]amino]- (9CI) (CA INDEX NAME)

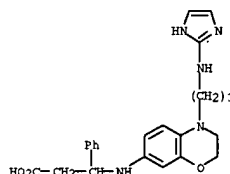


RN 511544-54-0 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[3-(1H-imidazol-2-ylamino)propyl]-2H-1,4-benzoxazin-7-yl]amino]- (9CI) (CA INDEX NAME)

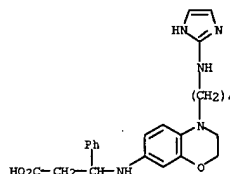
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L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



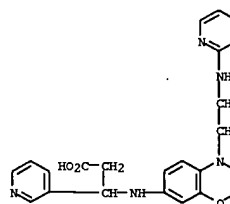
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CN Benzenepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[4-(1H-imidazol-2-ylamino)butyl]-2H-1,4-benzoxazin-7-yl]amino]- (9CI) (CA INDEX NAME)



RN 511544-58-4 CAPLUS

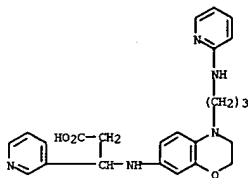
CN 3-Pyridinepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[2-(2-pyridinylamino)ethyl]-2H-1,4-benzoxazin-7-yl]amino]- (9CI) (CA INDEX NAME)



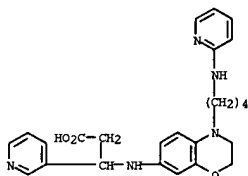
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L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
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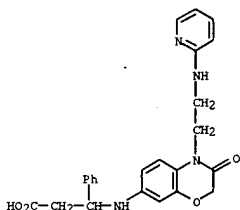


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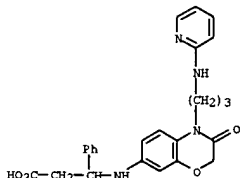


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L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 RN 511544-72-2 CAPLUS  
 CN Benzenepropanoic acid,  $\beta$ -[[[3,4-dihydro-3-oxo-4-[2-(2-pyridinylamino)ethyl]-2H-1,4-benzoxazin-7-yl]amino]- (9CI) (CA INDEX NAME)



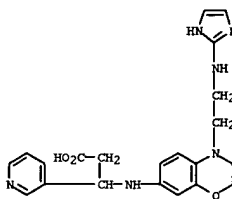
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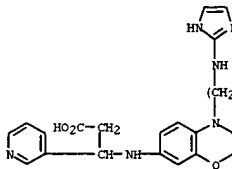
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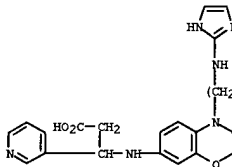
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



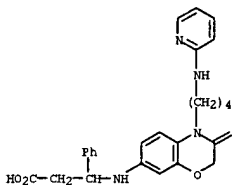
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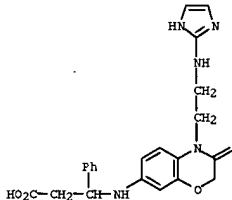
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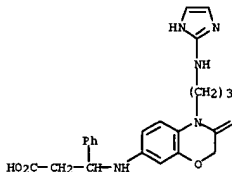
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 511544-80-2 CAPLUS  
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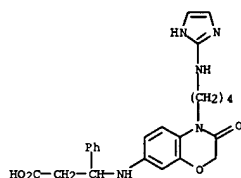


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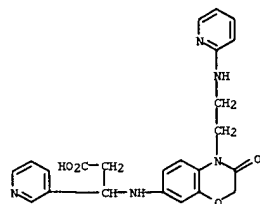


RN 511544-84-6 CAPLUS  
 CN Benzenepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[4-(1H-imidazol-2-

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
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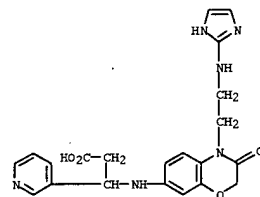


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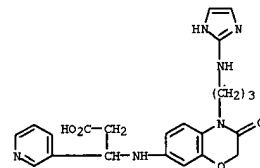


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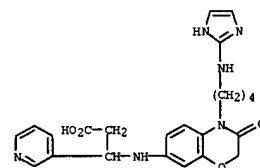
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



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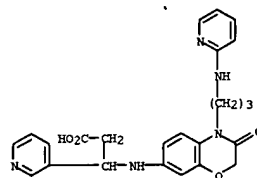
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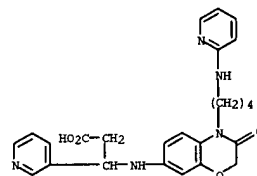
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L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

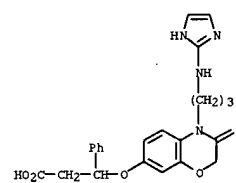


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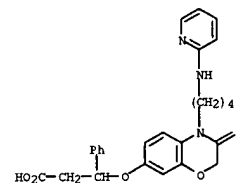


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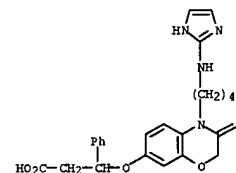
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



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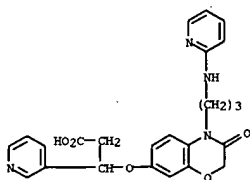
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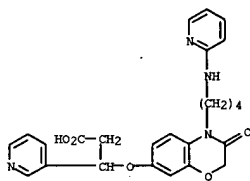
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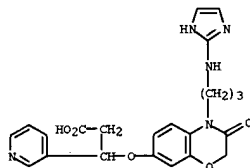
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



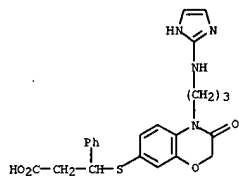
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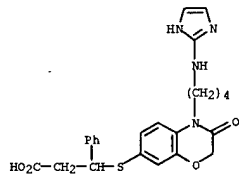
RN 511545-14-5 CAPLUS  
 CN 3-Pyridinepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[3-(1H-imidazol-2-ylamino)propyl]-3-oxo-2H-1,4-benzoxazin-7-yl]oxy]- (9CI) (CA INDEX NAME)



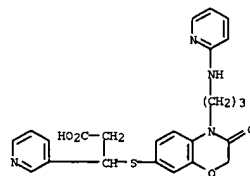
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 511545-25-8 CAPLUS  
 CN Benzenepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[4-(1H-imidazol-2-ylamino)butyl]-3-oxo-2H-1,4-benzoxazin-7-yl]thio]- (9CI) (CA INDEX NAME)



RN 511545-27-0 CAPLUS  
 CN 3-Pyridinepropanoic acid,  $\beta$ -[[[3,4-dihydro-3-oxo-4-[3-(2-pyridinylamino)propyl]-2H-1,4-benzoxazin-7-yl]thio]- (9CI) (CA INDEX NAME)

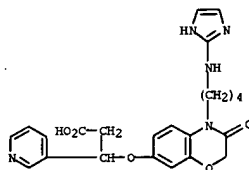


RN 511545-29-2 CAPLUS  
 CN 3-Pyridinepropanoic acid,  $\beta$ -[[[3,4-dihydro-3-oxo-4-[4-(2-pyridinylamino)butyl]-2H-1,4-benzoxazin-7-yl]thio]- (9CI) (CA INDEX NAME)

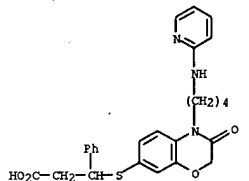
&lt;11/18/2005&gt;

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 511545-16-7 CAPLUS  
 CN 3-Pyridinepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[4-(1H-imidazol-2-ylamino)butyl]-3-oxo-2H-1,4-benzoxazin-7-yl]oxy]- (9CI) (CA INDEX NAME)

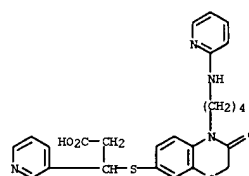


RN 511545-19-0 CAPLUS  
 CN Benzenepropanoic acid,  $\beta$ -[[[3,4-dihydro-3-oxo-4-[4-(2-pyridinylamino)butyl]-2H-1,4-benzoxazin-7-yl]thio]- (9CI) (CA INDEX NAME)

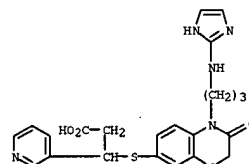


RN 511545-23-6 CAPLUS  
 CN Benzenepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[3-(1H-imidazol-2-ylamino)propyl]-3-oxo-2H-1,4-benzoxazin-7-yl]thio]- (9CI) (CA INDEX NAME)

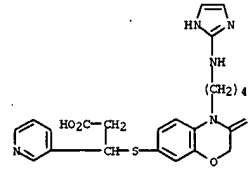
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 511545-31-6 CAPLUS  
 CN 3-Pyridinepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[3-(1H-imidazol-2-ylamino)propyl]-3-oxo-2H-1,4-benzoxazin-7-yl]thio]- (9CI) (CA INDEX NAME)



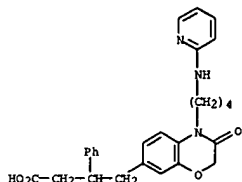
RN 511545-33-8 CAPLUS  
 CN Benzenepropanoic acid,  $\beta$ -[[[3,4-dihydro-4-[4-(1H-imidazol-2-ylamino)butyl]-3-oxo-2H-1,4-benzoxazin-7-yl]thio]- (9CI) (CA INDEX NAME)



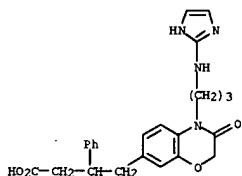
RN 511545-35-0 CAPLUS  
 CN 2H-1,4-Benzoxazine-7-butanolic acid, 3,4-dihydro-3-oxo- $\beta$ -phenyl-4-[4-(2-pyridinylamino)butyl]- (9CI) (CA INDEX NAME)

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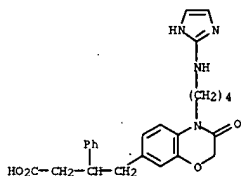
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 511545-37-2 CAPLUS  
 CN 2H-1,4-Benzoxazine-7-butanoic acid, 3,4-dihydro-4-[(1H-imidazol-2-ylamino)propyl]-3-oxo-β-phenyl- (9CI) (CA INDEX NAME)



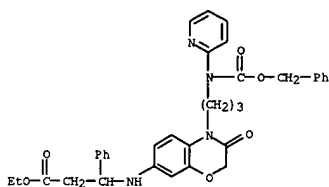
RN 511545-39-4 CAPLUS  
 CN 2H-1,4-Benzoxazine-7-butanoic acid, 3,4-dihydro-4-[(1H-imidazol-2-ylamino)butyl]-3-oxo-β-phenyl- (9CI) (CA INDEX NAME)



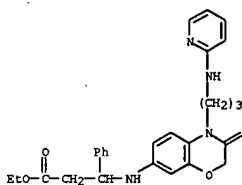
RN 511545-40-7 CAPLUS  
 CN 2H-1,4-Benzoxazine-7-butanoic acid, 3,4-dihydro-3-oxo-β-3-pyridinyl-4-[(1H-imidazol-2-ylamino)butyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

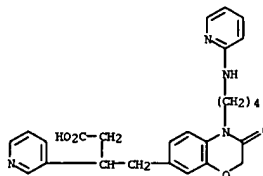
IT 511545-54-3P 511545-56-5P 511545-57-6P  
 511545-58-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of benzoxazines as integrin antagonists)  
 RN 511545-54-3 CAPLUS  
 CN Benzenepropanoic acid, β-[[[3,4-dihydro-3-oxo-4-[(2-pyridinylamino)propyl]-2H-1,4-benzoxazin-7-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



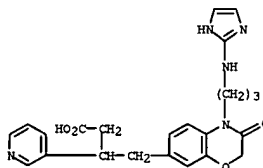
RN 511545-56-5 CAPLUS  
 CN Benzenepropanoic acid, β-[[[3,4-dihydro-3-oxo-4-[(2-pyridinylamino)propyl]-2H-1,4-benzoxazin-7-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



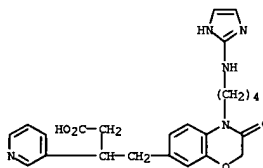
RN 511545-57-6 CAPLUS  
 CN Benzenepropanoic acid, β-[[[3,4-dihydro-4-[(3-(2-pyridinylamino)propyl)-1H-imidazol-2-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 [4-(2-pyridinylamino)butyl]- (9CI) (CA INDEX NAME)

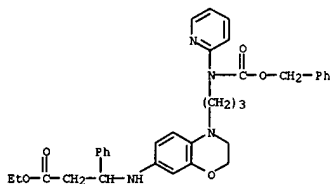
RN 511545-42-9 CAPLUS  
 CN 2H-1,4-Benzoxazine-7-butanoic acid, 3,4-dihydro-4-[(1H-imidazol-2-ylamino)butyl]-3-oxo-β-3-pyridinyl- (9CI) (CA INDEX NAME)



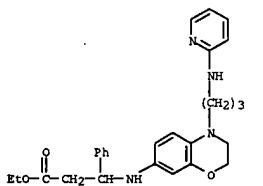
RN 511545-44-1 CAPLUS  
 CN 2H-1,4-Benzoxazine-7-butanoic acid, 3,4-dihydro-4-[(1H-imidazol-2-ylamino)butyl]-3-oxo-β-3-pyridinyl- (9CI) (CA INDEX NAME)



L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 511545-58-7 CAPLUS  
 CN Benzenepropanoic acid, β-[[[3,4-dihydro-4-[(3-(2-pyridinylamino)propyl)-2H-1,4-benzoxazin-7-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



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